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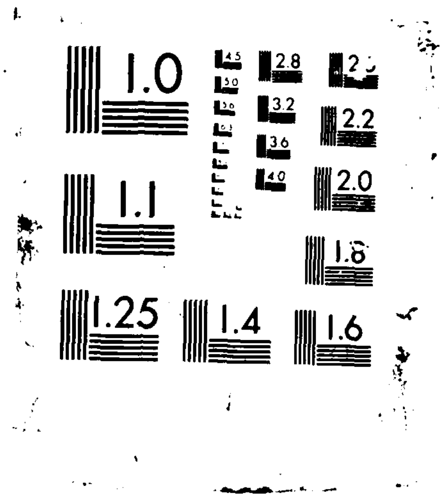
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Sung G. Chung and Thomas F. George

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Generalization of Levinson's Theorem to Particle-Matter Interactions

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Abstract

It is shown that Levinson's theorem in static potential scattering can be generalized to a particle dynamically interacting with one-dimensional matter systems (liquids or solids). A restriction on a particle-matter interaction is that it decays faster than an inverse quadratic of the particle-matter separation.

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1. Introduction

Levinson's theorem is one of the classic theorems in scattering theory. For s-wave motion of a par :le in a spherically-symmetric potential $V(r)$ in three dimensions, Levinson showed that the scattering phase shift $\delta(k)$ as a function of incident wave number k is related to the number of s-wave bound states N as

$$N = \delta(+0)/\pi \tag{1}$$

under certain conditions on the potential $V(r)$.[1,2] Jauch[3] and then Kazes[4] and Ida[5] later developed the method of scattering operator algebra, and succeeded to generalize the theorem to cases of nonlocal potentials. In this paper, we shall point out that the theorem can be generalized to the case of dynamical particle-matter interactions in one dimension (1-d).

A desire for this generalization arose in the course of our recent study of low-temperature adsorption of atoms on a material surface.[6] Consider a scattering eigenstate characterized by two wave numbers k_x and k_z of the incident particle as shown in Fig. 1a (the particle motion is in the xz-plane). The scattering wave function takes an asymptotic form at $z \to \infty$ of

$$|k^+\rangle \sim \phi_0\, e^{ik_x x}\left(e^{-ik_z z} - S(k_x,k_z)e^{ik_z z}\right) \quad , \tag{2}$$

where ϕ_0 represents the matter ground state ($T = 0$ K for simplicity, and we assume that the ground state is non-degenerate), and the S-matrix element $S(k_x,k_z)$ is in general a function of both k_x and k_z. Sometimes $S(k_x,k_z)$ has a weak k_x-dependence, whereby the problem becomes essesntially one-dimensional. One such example is found in recent experiments for ^{4}He atom scattering from a liquid ^{4}He surface, reporting a weak k_x-dependence for the reflectance coefficient as a function of k_x and k_z.[7] Indeed, previously people mainly considered a simplified 1-d model of particle-matter interactions to study low-temperature adsorption (cf. Fig. 1b). We note that a 1-d model must be of finite size, because otherwise the matter does not have a well-defined boundary at finite temperatures, and the question of calculating, for example, the adsorption probability of a particle becomes meaningless.[8]

A long-standing controversy in low-temperature adsorption based on a finite 1-d model concerns the importance of correlated motions of a particle near a material surface.[9,10] This is essentially a question on the importance of many-body effects. We thus encounter an interesting question: is it possible to dynamically generalize Levinson's theorem? In this paper, we shall show that there indeed exists a dynamical version of Levinson's theorem. The only restriction in our arguments is that the potential created by a matter system and seen by a particle must decay faster than an inverse quadratic of the particle-matter separation. We also assume that the ground state of the matter system is non-degenerate, which in fact is very likely the case for a finite system without a special symmetry.

We have organized the present paper as follows: In the next section, as a natural generalization of the static case,[1,11] we describe a scattering eigenstate of a finite 1-d model, particularly a Jost function and its general aspects. In Section 3, we discuss analytic properties of the Jost solution and Jost function. To do this, again as a natural generalization of the static case,[11,12] we consider an integral Schrödinger equation for the Jost solution, and its formal solution in terms of Fredholm series. A dynamical generalization of Levinson's theorem is then straightforward (Section 4). Finally in Section 5, our conclusion is given.

2. Scattering Eigenstate

The Hamiltonian for a particle interacting with a matter system is written in general as

$$H_{tot} = H(\bar{X},\bar{P}) + V(\bar{X},x) + K(p) \quad , \tag{3}$$

where $(\bar{X},\bar{P})$ are vector operators describing the positions and momenta of the matter atoms, and (x,p) describe the position and momentum of the particle. $H(\bar{X},\bar{P})$ is a 1-d matter Hamiltonian, $K(p)$ is the kinetic energy of the particle, and $V(\bar{X},x)$ describes the interaction between the particle and the 1-d matter system. Let us use the notations $\tilde{r} \equiv (\bar{X},x)$, m = mass of particle, and $\phi_0(\bar{X})$ and E_0, respectively, for the ground state of $H(\bar{X},\bar{P})$ ($T = 0$ K) and its energy. For a given total energy $E(k) = E_0 + \hbar^2k^2/2m$, the Schrödinger equation

$$H_{tot}\psi(\tilde{r},k) = E(k)\psi(\tilde{r},k) \tag{4}$$

has two independent solutions $F(\tilde{r},\pm k)$ with the asymptotic properties at $x \to \infty$

$$F(\tilde{r},\pm k) \to \phi_0(\bar{X})e^{\mp ikx} \quad . \tag{5}$$

The scattering state $\psi(\tilde{r},k)$ is then given as a linear combination of the Jost solutions $F(\tilde{r},\pm k)$. Noting that (4) is real and $\psi(\tilde{r},k)$ is an even function of k, we can write in general

$$\psi(\tilde{r},k) = \frac{i}{2k}[f(-k)F(\tilde{r},k) - f(k)F(\tilde{r},-k)] \quad . \tag{6}$$

To determine the Jost function $f(k)$ in the static case, one imposes the condition

$$\psi(x = x_0,k) = 0 \quad , \tag{7}$$

which is a requirement that the particle cannot reach the point $x = x_0$ where the potential energy is large. The corresponding physical condition in our dynamic case is that

$$\psi(\tilde{r} = \tilde{r}_c, k) = 0 \quad , \tag{8}$$

where $\tilde{r}_c$ is a constant vector independent of k. With a suitable choice of normalization, one can then take the Jost function f(k) as

$$f(k) = F(\tilde{r}_c, k) \quad . \tag{9}$$

A remark here is that the vectors $\tilde{r}_c$ which satisfy the condition (8) generally form a hypersurface. A consistent situation, therefore, is that by choosing the Jost function as (9) for a special point $\tilde{r} = \tilde{r}_c$ on the hypersurface, the condition (8) must be automatically satisfied for all the other points on the hypersurface. In other words, the Jost solutions $F(\tilde{r}, \pm k)$ must be strongly correlated.

In the next section, we shall examine an analytic property of the Jost solution $F(\tilde{r}, k)$ in the complex k-plane, which leads to the same analytic property of the Jost function f(k) due to (9). Before doing so, let us mention some general properties of f(k). First, it is seen from (5) and (6) that the zeroes of the Jost function f(k) on the negative imaginary axis in the complex k-plane describe the bound states of H_{tot}. In this paper, we restrict ourselves to those particle-matter potentials which decay faster than an inverse quadratic of the particle-matter separation. For such potentials, one can readily see that the number of bound states is finite, and therefore, except for physically uninteresting accidental situations,

$$f(0) \neq 0 \quad . \tag{10}$$

Second, the reality of H_{tot} means that

$$H_{tot}F^*(\tilde{r},-k^*) = E(k)F^*(\tilde{r},-k^*) \quad , \tag{11}$$

but since $F^*(\tilde{r},-k^*) \sim \phi_0(\tilde{X})e^{-ikx}$ as $x \to \infty$, we have

$$F^*(\tilde{r},-k^*) = F(\tilde{r},k) \quad . \tag{12}$$

Now since $\psi(\tilde{r},k)$ as given by (6) is a real, even function of k,

$$\psi^*(\tilde{r},k^*) = \psi(\tilde{r},k) \quad . \tag{13}$$

From (6), (12) and (13), we obtain the well-known relationship

$$f^*(-k^*) = f(k) \quad . \tag{14}$$

For real k, in particular, upon writing the Jost function as

$$f(k) = |f(k)|e^{i\delta(k)} \quad , \tag{15}$$

where $\delta(k)$ is a scattering phase shift, (10) and (14) give

$$-\delta(-k) = \delta(k) \tag{16}$$

under the convention that $\delta(\pm\infty) = 0$. A note on (16) is that $\delta(\pm\infty)$ need not be the same, so that they are not necessarily zero.

3. Analyticity of the Jost Function

We now discuss an analytic property of the Jost solution in the complex k-plane, leading to the same analytic property of the Jost function due to (9). Let us consider the following integral Schrödinger equation for $F(\tilde{r},k)$:

$$F(\tilde{r},k) = F_0(\tilde{r},k) + \int d\tilde{r}'\ K(\tilde{r},\tilde{r}';k)\ F(\tilde{r}',k) \quad , \tag{17}$$

where the integral kernel is

$$K(\tilde{r},\tilde{r}';k) \equiv -G(\tilde{r},\tilde{r}';k)V(\tilde{r}') \quad , \tag{18}$$

$V(\tilde{r}) \equiv V(\tilde{X},x)$, $F_0(\tilde{r},k) \equiv \phi_0(\tilde{X})e^{-ikx}$, and the Green's function $G(\tilde{r},\tilde{r}';k)$ is defined by

$$[H(\tilde{X},\tilde{P}) + K(p) - E(k)]G(\tilde{r},\tilde{r}';k) = \delta(\tilde{r} - \tilde{r}') \quad . \tag{19}$$

Introducing an orthonormal complete basis set $\{\phi_i(\tilde{X})\}$ for the matter Hamiltonian $H(\tilde{X},\tilde{P})$, we can write the Green's function G as

$$G(\tilde{r},\tilde{r}';k) = \sum_i \int \frac{dk'}{2\pi} \frac{e^{ik'(x-x')}}{E(i) + k'^2 - k^2 + i\varepsilon} \phi_i(\tilde{X})\phi_i^*(\tilde{X}') \quad , \tag{20}$$

where $E(i)$ is the energy difference between the states $\phi_i(\tilde{X})$ and $\phi_0(\tilde{X})$, and we have put $\hbar^2/2m = 1$. In (20) we have added the term $i\varepsilon$ (ε = infinitesmal positive number) in the denominator to describe an outgoing wave.

In carrying out the k'-integration in (20), as will become clear below, we need only consider k in the region D surrounded by the contour C: $[-k_0,k_0]$, $[k_0,k_0-i\infty]$, $[k_0-i\infty,-k_o-i\infty]$ and $[-k_0-i\infty,-k_0]$, where k_0 is an infinitesmal positive number. On the other hand, our 1-d matter is finite, and thus the excitation above the ground state has a gap, that is, $E(i) > 0$. Therefore, for k in the region D, it is always realized that

$$E(i,k) \equiv [E(i) - k^2]^{1/2} > 0 \quad . \tag{21}$$

With (21) in mind, we perform a contour integral over k' to obtain

$$G(\tilde{r},\tilde{r}';k) = \sum_i \frac{e^{-E(i,k)|x-x'|}}{2E(i,k)} \phi_i(\tilde{X})\phi_i{}^*(\tilde{X}') \quad . \tag{22}$$

The integral equation (17) can be solved formally by the Fredholm method:[13]

$$F(\tilde{r},k) = F_0(\tilde{r},k) + \frac{1}{\Delta}\int d\tilde{r}'\ \Delta(\tilde{r},\tilde{r}')F_0(\tilde{r}',k) \quad , \tag{23}$$

where

$$\Delta = 1 + \sum_{n=1}^{\infty} \frac{(-)^n}{n!}\int d\tilde{r} \ldots \int d\tilde{r}_n \quad \begin{matrix} K_{11} & \cdots & K_{1n} \\ \vdots & & \vdots \\ K_{n1} & \cdots & K_{nn} \end{matrix} \tag{24}$$

where $K(\tilde{r}_i,\tilde{r}_j)$ is abbreviated as K_{ij} and

$$\Delta(\tilde{r},\tilde{r}') = K(\tilde{r},\tilde{r}') + \sum_{n=1} \frac{(-)^n}{n!}\int d\tilde{r}_1 \ldots \int d\tilde{r}_n \begin{pmatrix} K_{rr'} & K_{r1} & \cdots & K_{rn} \\ K_{1r'} & K_{11} & \cdots & K_{1n} \\ \vdots & \vdots & & \vdots \\ K_{nr'} & K_{n1} & \cdots & K_{nn} \end{pmatrix} . \tag{25}$$

We note that both $F_0(\tilde{r},k)$ and the kernel $K(\tilde{r},\tilde{r}')$, as given by (18) and (22), are analytic in the region D. Therefore, if the Fredholm series in (24) and (25) converge, we reach the conclusion that the Jost solution $F(\tilde{r},k)$ as given by (23) is also analytic in the region D.

We now show the convergence of Δ. In a similar way, we can show the convergence of $\Delta(\tilde{r},\tilde{r}')$. We first note that from (18) and Hadamard's inequality [14] we can write

$$\begin{aligned} &\int d\tilde{r}_1 \ldots \int d\tilde{r}_n \det_{1\le i,j\le n} ||k_{ij}|| \\ &\le \int dx_1 \ldots \int dx_n \int d\tilde{X}_1 \ldots \int d\tilde{X}_n\ |V(\tilde{r}_1) \ldots V(\tilde{r}_n)| \cdot ||g_1|| \ldots ||g_n|| \quad , \end{aligned} \tag{26}$$

where $||g_i||$ is the norm of the i-th column vector of the matrix G_{ij}. Next, since our k is in the low-energy region D, the excitation of the matter from its ground state $\phi_0(\tilde{X})$ is limited to a finite number of low-lying excited states, i.e., with some integer I, (22) gives

$$|G_{rr'}| \leq \sum_{i<I} \frac{|\phi_i(\tilde{X})\phi_i(\tilde{X}')|}{2E(i,k)} \quad . \tag{27}$$

The wave functions of low-lying excited states are well localized in the $\tilde{X}$-space, and therefore, when carrying out the integrations $\int d\tilde{X}_1 \ldots \int d\tilde{X}_n$ in (26), one can apply the average-value theorem. This means that there exists a certain constant vector $\tilde{X}_0$ and finite constants A and B such that

$$\begin{aligned}
&\int d\tilde{X}_1 \ldots \int d\tilde{X}_n \, |V(\tilde{r}_1) \ldots V(\tilde{r}_n)| \cdot ||g_1|| \ldots ||g_n|| \\
&= |V(\tilde{X}_0,x_1)| \ldots |V(\tilde{X}_0,x_n)| \int d\tilde{X}_1 \ldots \int d\tilde{X}_n \, ||g_1|| \ldots ||g_n|| \\
&\leq |V(\tilde{X}_0,x_1)| \ldots |V(\tilde{X}_0,x_n)| \, A^n (Bn^{1/2})^n \quad .
\end{aligned} \tag{28}$$

Physically, $\tilde{X}_0$ describes a most probable configuration of the matter atoms at low temperatures. We finally note that since our $|V(\tilde{X}_0,x)|$ decays faster than x^{-2} at $x \to \infty$ by assumption,

$$\int dx \, |V(\tilde{X}_0,x)| \leq M < \infty \quad . \tag{29}$$

From (26), (28) and (29) we obtain

$$\int d\tilde{r}_1 \ldots \int d\tilde{r}_n \det_{1\leq i,j\leq n} ||K_{ij}|| \leq (MAB)^n \, n^{n/2} \quad , \tag{30}$$

which assures the convergence of Δ.

4. Dynamical Levinson's Theorem

In the preceding sections, we have discussed some general properties of the Jost function f(k) and its analytic property in the complex k-plane. We are now ready to claim the existence of dynamical Levinson's theorem in a similar manner as in the static potential scattering:

$$N_b = -\frac{1}{2\pi i}\int_C dk\,\frac{f'(k)}{f(k)} = -\frac{1}{2\pi i}\int_C d[\ln f(k)]$$

$$= -\frac{1}{2\pi}[\delta(-0) - \delta(+0)] = \delta(+0)/\pi \quad , \tag{31}$$

where N_b is the number of bound states of H_{tot}, and the contour C is as given in Fig. 2. This can be seen as follows: since the Jost function f(k) is analytic in the region D surrounded by the contour C, the integrand f'(k)/f(k) has simple poles of unit strength at zeroes of f(k), each of which corresponds to a bound state. For q degenerate bound states, the strength of the corresponding pole is q. This is the first equality in (31). The remaining equalities in (31) are trivial from (10), (15), (16) and the analyticity of f(k) in the region D.

5. Conclusion

In this paper, we have considered a 1-d model which describes a particle dynamically interacting with a finite 1-d matter. We have shown that if the matter has a non-degenerate ground state and is well-localized in space, and hence the collision of the particle with the matter is well-defined, and if the particle-matter potential decays faster than an inverse quadratic of the distance, there exists a dynamical version of Levinson's theorem, connecting the zero-energy phase shift δ(+0) to the number of bound states of the total system. This dynamical Levinson's theorem has recently played an essential role in the study of low-temperature adsorption.[6] Furthermore, in light of its general, many-body character, we expect its fruitful applications in other physical problems.

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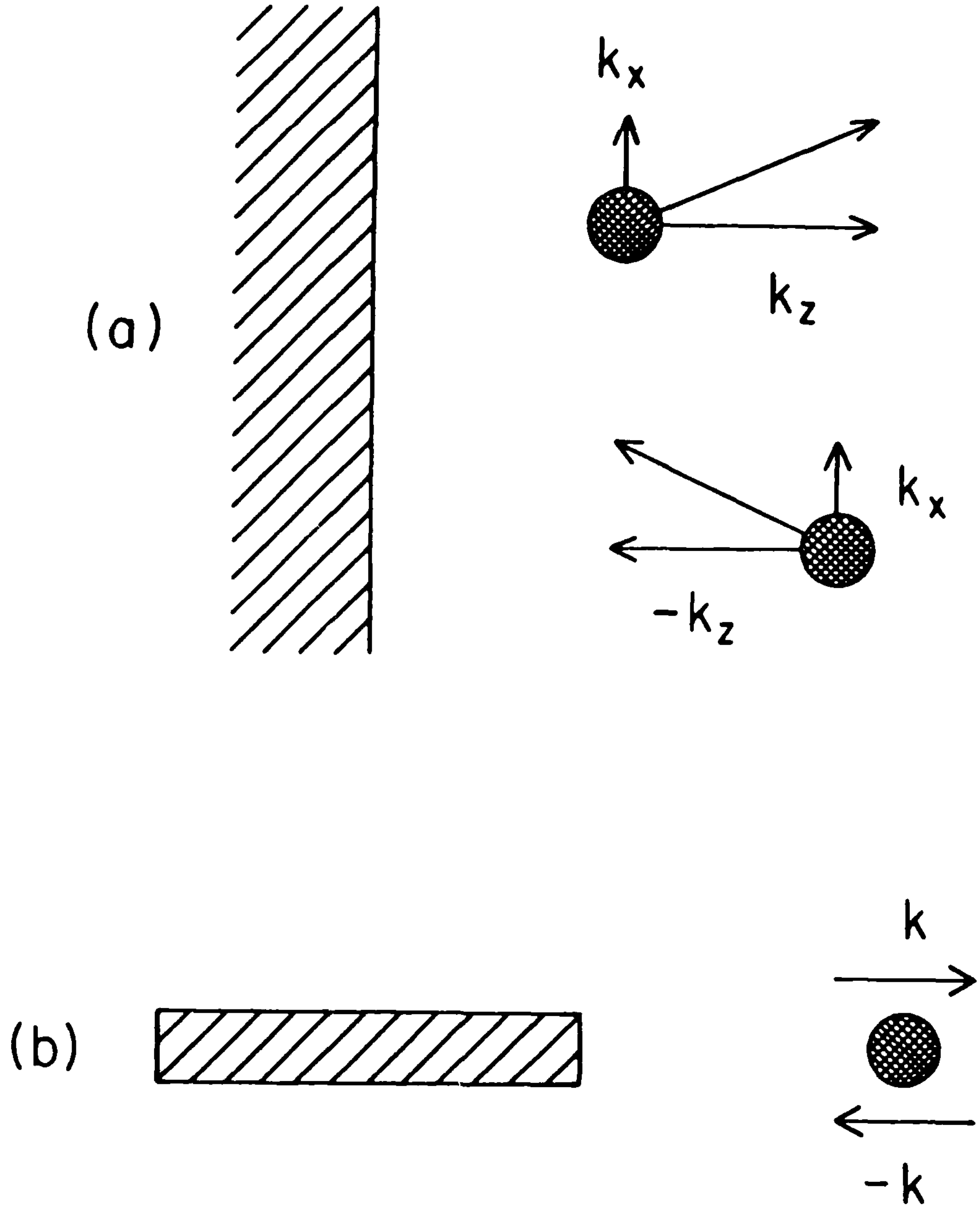
Figure Captions

Fig. 1 (a) Three-dimensional geometry for the scattering eigenstate characterized by the parallel and perpendicular wave numbers, k_x and k_z.

(b) Its one-dimensional simplification when the parallel and perpendicular motions are approximately separable.

Fig. 2 The contour C in the integral of (31). The crosses on the negative imaginary axis denote the zeroes of the Jost function f(k).



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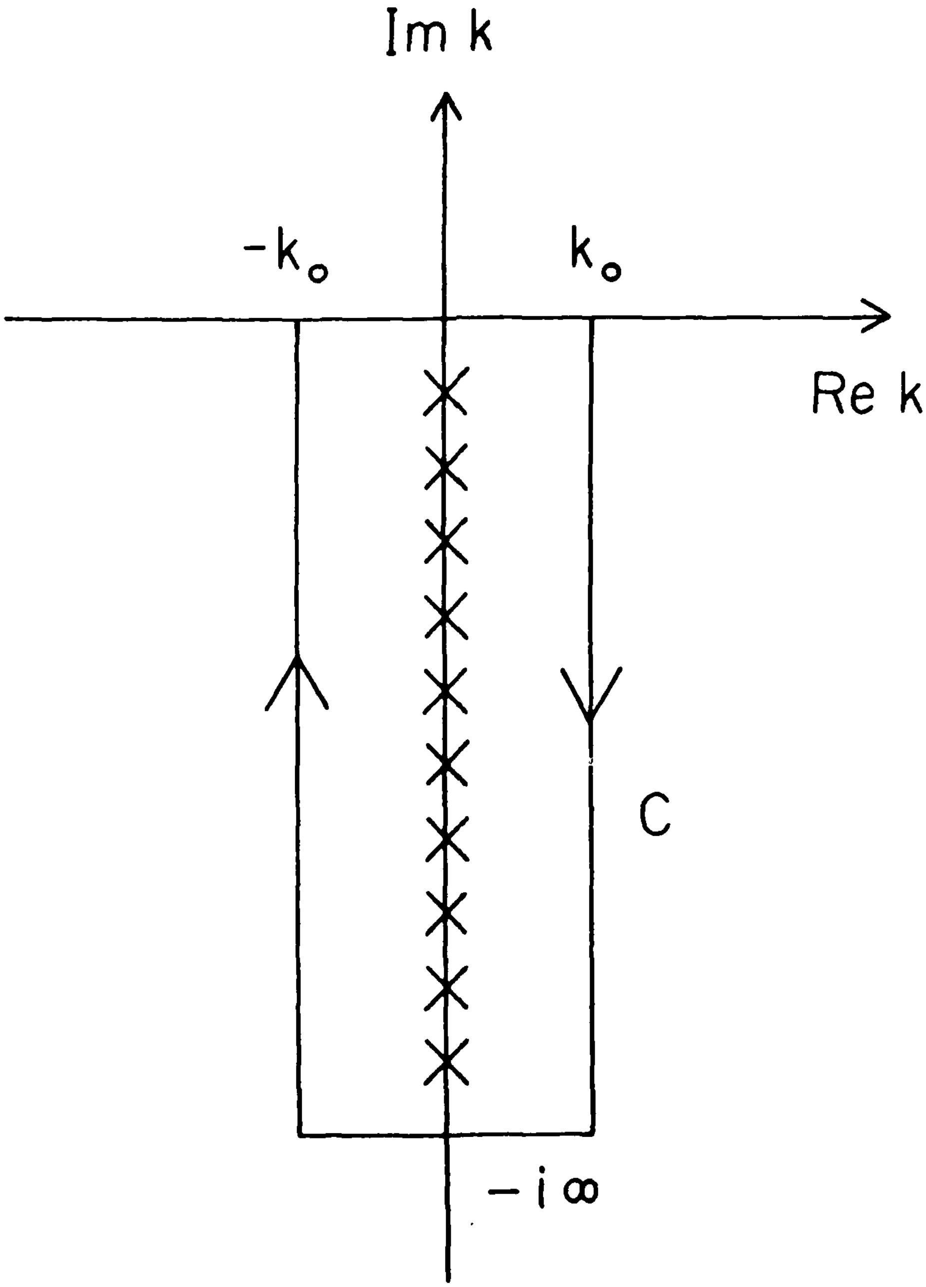

Fig. 2

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